

Theory for Slightly Doped Antiferromagnetic Mott Insulators

T. K. Lee^{1,2}, Chang-Ming Ho², Naoto Nagaosa^{3,4} and Wei-Cheng Lee¹

¹ *Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan 11529*

² *Physics Division, National Center for Theoretical Sciences, P.O.Box 2-131, Hsinchu, Taiwan*

300

³ *Department of Applied Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656,*

Japan

⁴ *Correlated Electron Research Center, AIST, Tsukuba, Ibaraki 303-0046, Japan*

(September, 2002. For the MOS2002 proceedings.)

Abstract

Trial wavefunctions, constructed explicitly from the unique 2-dimensional Mott insulating state with antiferromagnetic order, are proposed to describe the low-energy states of a Mott insulator slightly doped with holes or electrons. With the state behaving like charged quasi-particles with well-defined momenta, a rigid band is observed. These states have much less pairing correlations than previously studied ones. Small Fermi patches obtained are consistent with recent experiments on high T_c cuprates doped lightly with holes or electrons. States showing the incoherent and spin-bag behaviors are also discussed. Using these wavefunctions, a number of results obtained by exact calculations are reproduced.

PACS: 74.72.Jt, 75.50.Ee, 79.60.-i

With the continuous improvement of experimental technique and sample making, it has recently become possible to study in detail the phenomena in the lightly doped high T_c cuprates. Indeed, many intriguing behaviors concerning the physics of doping the two-dimensional(2D) Mott insulator in this very undoped regime are observed. Recent angle-resolved photoemission spectroscopy (ARPES) results unearth contrasting behaviors between lightly hole-doped $Ca_{2-z}Na_zCuO_2Cl_2$ (Na -CCOC) [1] and electron-doped $Nd_{2-x}Ce_xCuO_2$ (NCCO) high T_c cuprates [2]. Although ARPES on the undoped (*i.e.* $z=x=0$) insulating state shows an identical energy dispersion of a single hole created below the charge gap, results at a little higher dopings are demonstrated to be different: while a small hole patch is observed to be centered clearly at momentum $(\pi/2, \pi/2)$ in the Na -CCOC at even $z=0.1$, small electron patches centered at $(\pi, 0)$ and $(0, \pi)$ are observed for $x=0.04$ in NCCO. Moreover, the in-plane transport in lightly doped systems shows high mobility of the charge carriers [3]. This and the recent high-resolution scanning tunneling microscopy/spectroscopy results indicate the signature of the *quasi-particle* behavior [4].

The single hole/electron behavior and its dispersion have been studied using various approaches on the t - t' - t'' - J model [5,6,7,8,9,10]. However, these studies on doping holes and electrons into the system only emphasize the *asymmetry* resulting from the different signs of t' and t'' for the corresponding Hamiltonians. It is unclear whether the same physics is working for these two systems with *different* Hamiltonians. Should one try to construct a different theory when electron-doped cuprates are considered? Furthermore, do the models predict small Fermi surfaces and quasi-particles?

There are other issues concerning the model itself which have been bothersome. The studies applying the projected d -wave superconducting, or the resonating-valence-bond (RVB), state with the antiferromagnetic long range order (AFLRO) also suggest that away from half-filling, the superconductivity (SC) revives and the ground state shows both SC and AFLRO [13,14]. But so far most experiments do not support the coexistence. In addition, there has been not enough understanding on various properties found in the exact results of the t - J type models on finite clusters [5,6,8,9,10,11,12] in terms of the many-particle wave

functions (WF's).

In this paper, we discuss our recent proposal of a theory based on the variational approach to understand these issues [15,16]. Specific trial wavefunctions (TWF's) are constructed to describe both the low-energy states of the associated t - t' - t'' - J models with lightly doped holes and electrons. These WF's are generalizations of the single-hole WF first written down by Lee and Shih [7]. In contrast to other TWF's [17], ours are constructed solely from the optimized one at half-filling and include no hopping amplitudes t' and t'' . Yet, surprisingly, a number of properties including dispersion relations, momentum distributions, spectral weight *etc.* are obtained correctly for both hole-doped and electron-doped systems. In the following, the *Lee-Shih* WF for one doped hole is used and generalized for several holes as well as electron-doped systems. All numerical results reported below are from variational Monte Carlo (VMC) calculations for an 8×8 lattice with periodic boundary conditions.

At half-filling, the system is described by the Heisenberg Hamiltonian

$$\mathcal{H}_J = J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j), \quad (1)$$

where $\langle i, j \rangle$ denotes nearest-neighbor (*n.n.*) sites. Each site is occupied by only one single electron. As holes or electrons are doped into the system, we consider the Hamiltonian $\mathcal{H} = \mathcal{H}_{t-t'-t''} + \mathcal{H}_J$ including *n.n.* and longer range hoppings. Here $\mathcal{H}_{t-t'-t''} = -t \sum_{\langle i,j \rangle \sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} - t' \sum_{\langle i,l \rangle \sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{l\sigma} - t'' \sum_{\langle i,m \rangle \sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{m\sigma} + \text{H.c.}$ with $\langle i, l \rangle$ and $\langle i, m \rangle$ representing the second *n.n.* and third *n.n.* site pairs. Note that $\tilde{c}_{i\sigma}$ in $\mathcal{H}_{t-t'-t''}$ creates different kind of *holes* from single-electron-occupied sites at half-filling: *empty holes* (0*e*-hole) for hole doping and *two-electron-occupied holes* (2*e*-hole) for electron doping [18]. Operator $\tilde{c}_{i\sigma}$ is actually equal to $c_{i\sigma}(1 - n_{i,-\sigma})$ or $c_{i,-\sigma}n_{i\sigma}$ for hole or electron doped case, respectively. Therefore, despite the constraints, states in the two cases are in one-to-one correspondence after a local transformation $c_{i\sigma} \rightarrow c_{i,-\sigma}^\dagger$ is made. However, because of the Fermi statistics, the exchange of a single spin with a 2*e*-hole has an extra *minus* sign as compared to the 0*e*-hole. Hence, the only difference between the hole-doped and electron-doped t - t' - t'' - J model is $t'/t \rightarrow -t'/t$ and $t''/t \rightarrow -t''/t$ after we change the $c_{i\sigma}$ on B sublattice sites to $-c_{i\sigma}$ [5]. With all these,

we then treat the hole and electron doped cases in the same manner with the Lee-Shih WF originally proposed only for a single hole. The VMC results presented in this paper are for $J/t = 0.3$, $t'/t = -(+)0.3$ and $t''/t = +(-)0.2$ in the hole(electron) doped case following the values usually used [5].

We shall apply the standard VMC method [17] that enforces the local constraint exactly. Following the work by Lee and Shih [7], the TWF for one doped hole with momentum \mathbf{q} and $S_z=1/2$ is constructed to have $(N_s/2) - 1$ singlet pairs of electrons and a single unpaired electron with momentum \mathbf{q} and $S_z=1/2$,

$$|\Psi_1\rangle = P_d c_{\mathbf{q}\uparrow}^\dagger [\sum'_{\mathbf{k}} (A_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + B_{\mathbf{k}} b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger)]^{(N_s/2)-1} |0\rangle.$$

The prime on the summation symbol indicates that the momentum \mathbf{q} is excluded from the sum if \mathbf{q} is within the sublattice Brillouin zone (SBZ), otherwise, $\mathbf{q} - \mathbf{Q}$ is excluded. N_s here is the total number of sites and $\mathbf{Q}=(\pi, \pi)$.

$|\Psi_1\rangle$ is explicitly constructed from the optimized half-filled WF $|\Psi_0\rangle = P_d [\sum_{\mathbf{k}} (A_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + B_{\mathbf{k}} b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger)]^{N_s/2} |0\rangle$ and it does not contain any information about hoppings, t' , t'' and neither explicitly t , of the doped hole or electron. However, the effect of t is included in the RVB uniform bond $\chi = \langle \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} \rangle$ which describes the large quantum fluctuation and spin singlet formation. There is also no need to introduce t' and t'' in the TWF as they are compatible with AFLRO. Here the coefficients $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ are functions of $\xi_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$. $\pm \xi_{\mathbf{k}} = \pm (\epsilon_{\mathbf{k}}^2 + (Jm_s)^2)^{\frac{1}{2}}$ are energy dispersions for the two spin density wave (SDW) bands with $\epsilon_{\mathbf{k}} = -\frac{3}{4}J\chi(\cos k_x + \cos k_y)$ and the staggered magnetization $m_s = \langle S_A^z \rangle = -\langle S_B^z \rangle$, where the lattice is divided into A and B sublattices. $a_{\mathbf{k}\sigma}$ and $b_{\mathbf{k}\sigma}$ represent the operators of the lower and upper SDW bands, respectively, and are related to the original electron operators $c_{\mathbf{k}\sigma}$ and $c_{\mathbf{k}+\mathbf{Q}\sigma}$ with $\mathbf{Q}=(\pi, \pi)$ set for the commensurate SDW state. $\Delta_{\mathbf{k}} = \frac{3}{4}J\Delta d_{\mathbf{k}}$ with $d_{\mathbf{k}} = \cos k_x - \cos k_y$ here is for the d -wave RVB (d -RVB) order parameter. The projection operator P_d enforces the constraint of no doubly occupied (or vacant) sites for cases with finite hole (or electron) doping. At half-filling, N_s equals the total number of electrons. Notice that the sum in $|\Psi_0\rangle$ is taken over SBZ. There are two variational parameters: Δ/χ

and m_s/χ in these WF's.

The energy dispersion obtained from $|\Psi_1\rangle$ for one doped hole has been shown by Lee and Shih [7] to agree very well with that of exact calculations, self-consistent Born approximations (SCBA), and Green function Monte Carlo methods *etc.*. As for the case of having an extra up-spin electron with momentum \mathbf{q} doped into the half-filled state, the energy dispersion can be calculated with this same WF $|\Psi_1\rangle$. The only difference is signs of t'/t and t''/t are changed in the Hamiltonian.

The variational energies for one doped electron are shown as black dots in Fig.1. This result agrees well with that of Xiang and Wheatley [6] obtained by SCBA. The optimal variational parameters are $(\Delta/\chi, m_s/\chi)=(0.25, 0.125)$. The ground state is at momentum $\mathbf{q} = (\pi, 0)$. The VMC results can be fitted simply by $E_{1\mathbf{k}} = E_{\mathbf{k}} - 2t_{eff}(\cos k_x + \cos k_y) - 4t'_{eff}\cos k_x \cos k_y - 2t''_{eff}(\cos(2k_x) + \cos(2k_y))$ with parameters described in the caption of Fig.1. The dispersion thus seems to be simply the combination of the mean-field band at half-filling and the coherent hoppings [7].

To examine further the physical properties of $|\Psi_1\rangle$, we calculated the momentum distribution function $\langle n^h_{\sigma}(\mathbf{k}) \rangle$ for the ground state of a single hole with momentum $\mathbf{q} = (\pi/2, \pi/2)$ and $S_z=1/2$. Results are shown in Fig.2(a) and (b). Note that the dips or pockets at $(\pi/2, \pi/2)$ and *anti-dips* at $(-\pi/2, -\pi/2)$ found by Leung [10] for the exact results of 32 sites are also clearly seen here. It is quite amazing that $|\Psi_1\rangle$, including no t' and t'' , not only produces the correct energy dispersions for a single doped hole or electron it also provides a correct picture about the momentum distribution.

The momentum distribution functions $\langle n^e_{\sigma}(\mathbf{k}) \rangle$ for electron doped systems could be also calculated from $|\Psi_1\rangle$ if we perform the transformation, $c_{i\sigma} \rightarrow c_{i,-\sigma}^{\dagger}$, and t is chosen to be positive. In fact, it is easy to show that $\langle n^e_{\sigma}(\mathbf{k}) \rangle = 1 - \langle n^h_{-\sigma}(\mathbf{Q} - \mathbf{k}) \rangle$. The results for the ground state of a single doped electron with momentum $\mathbf{k} = (\pi, 0)$ and spin $S_z=1/2$ are shown in Fig.2(c) and (d). There are peaks at $\mathbf{k} = (\pi, 0)$ and an *anti-peak* at $\mathbf{k} = (0, \pi)$.

Now we shall generalize the Lee-Shih WF $|\Psi_1\rangle$ to the case of two holes. The simplest possible way is just to take out the unpaired spin from $|\Psi_1\rangle$ if we are interested in the state

with zero total momentum and $S_z=0$, which turns out to be the lowest energy state. The TWF for two holes with momenta \mathbf{q} and $-\mathbf{q}$ is

$$|\Psi_2\rangle = P_d [\sum_{\mathbf{k}}' (A_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + B_{\mathbf{k}} b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger)]^{(N_s/2)-1} |0\rangle.$$

Note that the momentum \mathbf{q} is not included in the summation. It is most surprising to find that although $|\Psi_2\rangle$ has zero total momentum irrespective of \mathbf{q} , its energy varies with the missing momentum or *the hole momentum* \mathbf{q} . The dispersion turns out to be very similar to that of a single electron as shown in Fig.1 [15]. The state with momentum $\mathbf{q}=(\pi, 0)$ has the lowest energy for two electrons. The values of the two parameters Δ/χ and m_s/χ are the same for $|\Psi_2\rangle$ and $|\Psi_1\rangle$.

Using WF $|\Psi_2\rangle$, the energy dispersion for two holes doped into the half-filled state again has an almost identical form as that of a single hole and the minimum is at $\mathbf{q} = (\pi/2, \pi/2)$ [7]. The lowest energy obtained is $-26.438(3)t$ which is much lower than the variational energy, $-25.72(1)t$, using the TWF applied by Himeda and Ogata [14]. Even if we include t' and t'' , the variational energy $-25.763(7)t$, is still much higher than ours [19]. We also found that the hopping amplitudes for *n.n.*, second *n.n.* and third *n.n.* of two holes are almost twice that of one hole. The momentum distribution function for this state (not shown) has dips at $(\pi/2, \pi/2)$ and $(-\pi/2, -\pi/2)$. This is in good agreement with the exact result [10] for the t - t' - t'' - J model with 2 holes in 32 sites.

It is then straightforward to write down the same type of TWF for three holes with momenta \mathbf{q} , \mathbf{q}' and $-\mathbf{q}'$:

$$|\Psi_3\rangle = P_d c_{\mathbf{q}\uparrow}^\dagger [\sum_{\mathbf{k}}' (A_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + B_{\mathbf{k}} b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger)]^{(N_s/2)-2} |0\rangle,$$

where \mathbf{q}' and \mathbf{q} are excluded from the summation. Just like the case with two holes or two electrons energy dispersions are proportional to the sum of the three single hole energies at momenta \mathbf{q} , \mathbf{q}' and $-\mathbf{q}'$. In Fig.3, the dispersions are plotted as functions of \mathbf{q} . For the electron doped (*i.e.* with three $2e$ -holes) case in Fig.3(a), the lowest energy state is at $\mathbf{q} = (3\pi/4, 0)$ (shown as an open circle) within the SBZ after the first two electrons occupy

$\mathbf{q}' = (\pi, 0)$. With three doped holes (Fig.3(b)), after the two electrons at $(\pi/2, \pi/2)$ are removed the ground state is now at $(\pi/2, -\pi/2)$ (the open circle). As shown clearly in Fig.3, the dispersions follow nicely the single hole one.

Values of the staggered magnetization $m = N_s^{-1} \sum_i (-1)^i S_i^z$ are computed and compared for several 0e-hole and 2e-hole concentrations. With the same variational parameters, it is found that the preference of $(\pi/2, \pi/2)$ for 0e-holes causes clearly larger disturbance of the AF order than for the electron doped case where 2e-holes with momentum $(\pi, 0)$ shows much less influence on the AF order [15]. This is consistent with previous work [5]. It is also consistent with experimental results that AF phase is more stable for electron doping than hole doping [20].

So far, based on the t - t' - t'' - J model we have proposed a TWF to describe the low energy states of slightly doped antiferromagnetic Mott insulators. Exactly the same TWF's are proposed to account for the behavior of both hole doping and electron doping, after we employed the particle-hole transformation. Different energy dispersions for these two cases are due to the different signs of t'/t and t''/t which is a direct consequence of the constraint that electron doped system has 2e-holes while hole doped system only has 0e-holes. Rigid band and *quasi-particle* behavior are demonstrated for both cases. The theory provides an explanation of recent ARPES results. In lightly hole-doped cuprates, small Fermi pocket is around $(\pi/2, \pi/2)$. In electron-doped cuprates, the patch is around $(\pi, 0)$ as shown in the inset of Fig.1 with doping at about 3%.

Another important property of our WF's is that holes are essentially independent of each other as they obey the same energy dispersions (with very little renormalization of parameters). Exactly because this quasi-particle like property is unchanged after doping, our WF has AFLRO but very little superconducting pairing correlations. The presence of superconducting state certainly will change the excitation spectra. In particular, the d -wave SC, which coexists with AFLRO in some of the previous variational studies, should have low energy excitations along the nodes. This is certainly not seen in our TWF's. In addition, the holes are not attractive to each other in our WF's. In Fig.4 the hole-hole correlation

function for our TWF and the WF used by authors in [14] are compared for 4 holes in an 8×8 lattice. The lack of attraction between holes is consistent with Leung's low energy states obtained exactly for two holes in 32 sites [10]. Long range d -wave pairing correlation defined [17] for our TWF and that in Himeda-Ogata one are, on average, about 0.002, and 0.018, respectively. Thus the d -RVB pairing for spins assumed by our WF's are not in any way implying the pairing of charges.

Although our TWF's or the Lee-Shih WF's has reproduced many numerical results obtained by exact diagonalization, SCBA, *etc.* for one or two holes or electrons, there exists, however, some inconsistency in the detail of the comparison. Namely, at some momenta \mathbf{k} 's the spectral weights $Z_{\mathbf{k}} = |\langle \Psi_{\mathbf{k}} | c_{\mathbf{k}\sigma} | \Psi_0 \rangle|^2 / \langle \Psi_0 | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} | \Psi_0 \rangle$ computed for the one doped hole case using $|\Psi_{\mathbf{k}}\rangle = |\Psi_1\rangle$ are much larger than the exact results [8]. This may indicate that the quasi-particle states do not exist everywhere in the Brillouin zone. In fact, the ARPES on the undoped ($z = 0$) *Na*-CCOC also show well-defined peaks only locally in the high-symmetry directions [1].

We have constructed TWF's with which small spectral weights are realized at particular \mathbf{k} points [16]. For the single hole doped case, state described by WF

$$|\Psi'_1\rangle = P_d c_{\mathbf{q}_s\uparrow}^\dagger \left[\sum_{[\mathbf{k} \neq \mathbf{q}_h]} (A_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + B_{\mathbf{k}} b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger) \right]^{(N_s/2)-1} |0\rangle$$

with the hole momentum $\mathbf{q}_h = (\pi/2, \pi/2)$ has also one singlet bond less than the half-filled case, but the unpaired spin momentum \mathbf{q}_s is chosen here not to be the same as \mathbf{q}_h . Note that only \mathbf{q}_h is excluded within the sum for $|\Psi'_1\rangle$. With the same parameters Δ/χ and m_s/χ , it is found that $|\Psi'_1\rangle$ can have *lower* variational energy than that of the quasi-particle state $|\Psi_1\rangle$ at some \mathbf{q}_s 's. Apparently, many states could be constructed with same \mathbf{q}_s but different \mathbf{q}_h . These states constitutes the continuum at *higher* energy.

Substituting WF $|\Psi'_1\rangle$ and the quasi-particle $|\Psi_1\rangle$ into $|\Psi_{\mathbf{k}}\rangle$ and computing $Z_{\mathbf{k}}$ suffices to reproduce the variation of the spectral weights obtained in the exact results [8]. States described by $|\Psi'_1\rangle$ have smaller $Z_{\mathbf{k}}$'s and are thus with a strong *incoherent* character. We also found that more quasi-particle states have lower energy below the continuum in the

pure t - J model with $t' = t'' = 0$ [11] than in the t - t' - t'' - J model. This is consistent with what has been known in the exact results [8].

To understand the incoherent states more, the hole-spin correlations for $|\Psi'_1\rangle$ with different \mathbf{q}_s 's are examined [16]. The spin configurations around the hole are quite different from that of the quasi-particle states. Spin moments around the hole in the quasi-particle state $|\Psi_1\rangle$ can have values larger than the average at that momentum, thus the unpaired spin seems to be bound to the hole. However, in the incoherent state the staggered magnetization is suppressed around the hole, this is like a spin-bag state [21]. The unpaired spin is no longer associated with the hole and this is now a spin-charge separated state. The amazing difference between these two wave functions could be understood quite easily. When we apply the spin flipping operator, $S^{\dagger(-)}(\mathbf{k}'; \mathbf{q}' = \mathbf{q}[\equiv \mathbf{q}_h]) = \sum_{\mathbf{q}'} c_{\mathbf{q}'+\mathbf{k}'\uparrow(\downarrow)}^\dagger c_{\mathbf{q}'\downarrow(\uparrow)} |_{\mathbf{q}'=\mathbf{q}}$ with $\mathbf{q}' + \mathbf{k}' = \mathbf{q}_s$, to the quasi-particle state, the unpaired spin \mathbf{q} is excited to a new momentum \mathbf{q}_s in the state $|\Psi'_1\rangle$. Thus the unpaired spin is no longer bound to the hole. Furthermore, the spin-spin correlations across the hole with $\mathbf{q}_s = (\pi, 0)$ show the *anti-phase* domain, *i.e.* AF correlation at the same sublattice. These features reproduce what have been obtained in the exact calculations [9].

In summary, we have discussed new TWF's describing the low-energy states of the t - t' - t'' - J model at lightly doping. These states reproduce various exact numerical results and, also, show consistent behaviors with what have been observed in the experiments.

We are grateful to Drs. A. Damascelli, F. Ronning and Prof. Z.-X. Shen for sharing their ARPES data prior to publication, and Profs. C.-T. Shih and P. W. Leung for some supporting results and invaluable discussions. TKL is supported by the grant NSC89-2112-M-001-103 (R.O.C.) and NN is supported by Priority Areas Grants and Grant-in-Aid for COE research from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

REFERENCES

- [1] A. Damascelli, Z. -X. Shen and Z. Hussain, cond-mat/0208504; F. Ronning *et al.*, Science **282**, 2067 (1998); Y. Kohsaka *et al.*, cond-mat/0209339; F. Ronning *et al.*, unpublished.
- [2] N. P. Armitage *et al.*, Phys. Rev. Lett. **88**, 257001 (2002).
- [3] For hole-doped systems, see, *e.g.*, Y. Ando, K. Segawa, A. N. Lavrov and S. Komiya, this proceeding; for electron-doped one, Y. Onose, Y. Taguchi, K. Ishizaka and Y. Tokura, Phys. Rev. Lett. **87**, 217001 (2001).
- [4] J. E. Hoffman, *et al.*, Science **297**, 1148 (2002); C. Howald *et al.*, cond-mat/0208442 .
- [5] T. Tohyama and S. Maekawa, Phys. Rev. B **49**, 3596 (1994); R. J. Gooding, K. J. E. Vos and P. W. Leung, Phys. Rev. B **50**, 12866 (1994).
- [6] T. Xiang and J. M. Wheatley, Phys. Rev. B **54**, R12653 (1996).
- [7] T. K. Lee and C. T. Shih, Phys. Rev. B **55**, 5983 (1997).
- [8] P. W. Leung, B. O. Wells and R. J. Gooding, Phys. Rev. B **56**, 6320 (1997).
- [9] T Tohyama *et al.*, J. Phys. Soc. Jpn. **69**, 9 (2000).
- [10] P. W. Leung, Phys. Rev. B **65**, 205101 (2002) and private communications.
- [11] P. W. Leung and R. J. Gooding, Phys. Rev. B **52**, R15711 (1995).
- [12] A. L. Chernyshev, P. W. Leung and R. J. Gooding, Phys. Rev. B **58**, 13594 (1998).
- [13] T. K. Lee, and S. P. Feng, Phys. Rev. B **38**, 11809 (1988); G. J. Chen *et al.*, Phys. Rev. B **42**, 2662 (1990).
- [14] A. Himeda and M. Ogata, Phys. Rev. B **60**, R9935 (1999).
- [15] T. K. Lee, C.-M. Ho and N. Nagaosa, unpublished.
- [16] W.-C. Lee, T. K. Lee and C.-M. Ho, unpublished.

- [17] For the introduction and early work of VWF study, see C. Gros, Ann. Phys. (New York) **189**, 53 (1989); also see, for the more recent, *e.g.*, H. Yokoyama and M. Ogata, J. Phys. Soc. Jpn. **65**, 3615 (1996).
- [18] D. G. Clarke, Phys. Rev. B **48**, 7520 (1993).
- [19] Actually, the lowest energy for Himeda-Ogata type TWF is obtained when its parameters are chosen to replicate our TWF. Details are to be reported elsewhere.
- [20] H. Takagi, Y. Tokura and S. Uchida, Physica C **162-164**, 1001 (1989); *ibid.*, Phys. Rev. Lett. **62**, 1197 (1989); G. M. Luke *et al.*, Phys. Rev. B **42**, 7981 (1990); K. Yamada *et al.*, J. Phys. Chem. Solids, **60**, 1025 (1999).
- [21] J. R. Schrieffer, X. G. Wen and S. C. Zhang, Phys. Rev. Lett. **60**, 944 (1988).

FIGURES

FIG. 1. Energy dispersion of one electron in the t - t' - t'' - J model on an 8×8 lattice. Black dots are VMC results by using $|\Psi_1\rangle$. The fitted dispersion $E_{1\mathbf{k}} - E_0$ are plotted as gray diamonds with parameters $\chi = 6.92$, $\Delta = 2.71$, $m_s = 18.84$, $E_0 = 7.43$, $t_{eff} = 0.06$, $t'_{eff} = -0.15$, $t''_{eff} = 0.1$. Inset: patches in one of BZ by filling the fitted dispersion in the main figure up to $\sim 3\%$ doping.

FIG. 2. Momentum distribution functions $\langle n_{\sigma}^{h(e)}(\mathbf{k}) \rangle$ for a single hole, (a) and (b), and electron, (c) and (d), in the 8×8 t - t' - t'' - J model. A scale is shown in between each set. The darker area indicates smaller values of $\langle n_{\sigma}^{h(e)}(\mathbf{k}) \rangle$.

FIG. 3. Energy dispersions of (a) three doped electrons and (b) three doped holes in the t - t' - t'' - J model. Filled circles are VMC results for the momenta shown along the horizontal axis by using $|\Psi_3\rangle$. A total minus sign has been multiplied to the hole doped case. Open circles, with the momenta also displayed, represent the lowest energy states. Results here are obtained with parameters shown in the figures.

FIG. 4. Hole-hole correlation functions with 4 doped holes in the 8×8 lattice. The result obtained using our WF, *i.e.* same form as $|\Psi_2\rangle$ with momenta $(\pi/2, \pi/2)$ and $(\pi/2, -\pi/2)$ excluded in the sum, is compared with that using the Himeda-Ogata WF. Results here are obtained with optimized parameters $(\Delta/\chi, m_s/\chi) = (0.25, 0.125)$ and, for Himeda-Ogata one, also $\mu = -0.025$.

This figure "1e-disp.jpg" is available in "jpg" format from:

<http://arXiv.org/ps/cond-mat/0210086v1>

This figure "3eh-disp.jpg" is available in "jpg" format from:

<http://arXiv.org/ps/cond-mat/0210086v1>

This figure "4h-hh.jpg" is available in "jpg" format from:

<http://arXiv.org/ps/cond-mat/0210086v1>

This figure "nk1-eh-c.jpg" is available in "jpg" format from:

<http://arXiv.org/ps/cond-mat/0210086v1>